

HOMOGENIZATION OF REACTION-DIFFUSION SYSTEMS

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Joint work with Grégoire Allaire & Laurent Desvillettes

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- ♣ These equations should model chemical species *reacting* with each other and *diffusing* in the spatial domain

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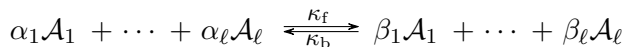
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- ♣ Supplemented by initial and boundary data

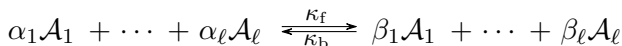
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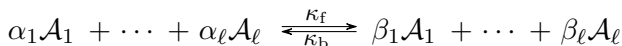
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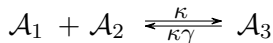


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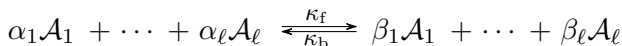
THREE SPECIES SYSTEM

- ♣ Take $(\alpha_1, \alpha_2, \alpha_3) = (1, 1, 0)$ and $(\beta_1, \beta_2, \beta_3) = (0, 0, 1)$



$$\mathcal{R}_1(u) = \mathcal{R}_2(u) = -\kappa(u_1 u_2 - \gamma u_3); \quad \mathcal{R}_3(u) = \kappa(u_1 u_2 - \gamma u_3)$$

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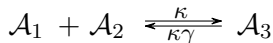


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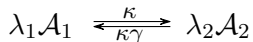
- ♣ Observe that $\mathcal{R}_1 + \mathcal{R}_3 = \mathcal{R}_2 + \mathcal{R}_3 = 0$

REVERSIBLE CHEMISTRY (CONTD.)

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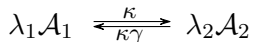


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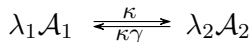
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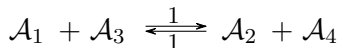


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FOUR SPECIES SYSTEM

♣ Take $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (1, 0, 1, 0)$ and $(\beta_1, \beta_2, \beta_3, \beta_4) = (0, 1, 0, 1)$

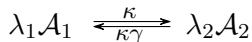


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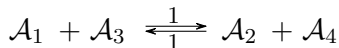


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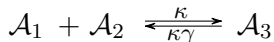


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WE PRESENT COMPUTATIONS FOR THREE SPECIES SYSTEM



$$\begin{cases} \partial_t u_1^\varepsilon - \operatorname{div} \left(d_1(x) \mathbf{D} \left(\frac{x}{\varepsilon} \right) \nabla u_1^\varepsilon \right) = -\frac{\kappa}{\varepsilon^2} (u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon) \\ \partial_t u_2^\varepsilon - \operatorname{div} \left(d_2(x) \mathbf{D} \left(\frac{x}{\varepsilon} \right) \nabla u_2^\varepsilon \right) = -\frac{\kappa}{\varepsilon^2} (u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon) \\ \partial_t u_3^\varepsilon - \operatorname{div} \left(d_3(x) \mathbf{D} \left(\frac{x}{\varepsilon} \right) \nabla u_3^\varepsilon \right) = \frac{\kappa}{\varepsilon^2} (u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon) \end{cases}$$

♣ Supplement with

- ▶ initial data
- ▶ zero Neumann boundary condition

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♣ Multiply rate functions by logarithms: for $i = 1, 2$,

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- ♣ Summing the expressions

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- ♣ Take the ordinary differential equations: $\dot{u}_i = \mathcal{R}_i(u)$
- ♣ Using logarithmic multipliers, the entropy dissipation inequality:

$$\frac{d}{dt} \sum_{i=1}^3 (u_i \log(u_i) - u_i + c) \leq 0$$

STRATEGY FOR HOMOGENIZATION

♣ The evolution equation:

$$\partial_t u_i^\varepsilon - \operatorname{div} \left(d_i(x) \mathbf{D} \left(\frac{x}{\varepsilon} \right) \nabla u_i^\varepsilon \right) = \frac{1}{\varepsilon^2} \mathcal{R}_i(u^\varepsilon) \quad \text{in } \Omega_T := (0, T) \times \Omega.$$

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♣ A typical homogenization result: for $\varepsilon \ll 1$,

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- ♣ A typical homogenization result: for $\varepsilon \ll 1$,

$$u_i^\varepsilon(t, x) \approx u_i^*(t, x) + \varepsilon \tilde{u}_i \left(t, x, \frac{x}{\varepsilon} \right)$$

- ♣ Characterize limit $u_i^*(t, x)$ as a solution to a differential equation.

LINEAR SETTING	NONLINEAR SETTING
Find uniform bounds on $u_i^\varepsilon(t, x)$ in $L^p((0, T); W^{1,p}(\Omega))$ for some $p > 1$ $u_i^\varepsilon \rightharpoonup u_i^*$ in $L^p((0, T); W^{1,p}(\Omega))$	$u_i^\varepsilon(t, x)$ relatively compact in $L^p(\Omega_T)$ for some $p > 1$ i.e. $\ u_i^\varepsilon - u_i^*\ _{L^p(\Omega_T)} \rightarrow 0$

BATTLE PLAN I

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BATTLE PLAN II

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- ♣ Limit problem couples parabolic problems with algebraic equation.
- ♣ Substitute algebraic relation to yield cross-diffusion interpretation.

BATTLE PLAN I – STEP 1

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Suppose the initial data $u_i^{\text{in}} \geq 0$.

Then the solution $u_i^\varepsilon(t, x) \geq 0$ in Ω_T

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- ♣ Integrate over Ω_t

BATTLE PLAN I – STEP 2

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$$\begin{aligned} \frac{d}{dt} \sum_{i=1}^3 \int_{\Omega} (u_i^\varepsilon \log(u_i^\varepsilon) - u_i^\varepsilon + c) dx + \sum_{i=1}^3 \int_{\Omega} |\nabla \sqrt{u_i^\varepsilon}|^2 dx \\ = -\frac{\kappa}{\varepsilon^2} \int_{\Omega} \left(u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon \right) \left(\log(u_1^\varepsilon u_2^\varepsilon) - \log(\gamma u_3^\varepsilon) \right) dx \leq 0 \end{aligned}$$

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♣ Integrating above expression over $(0, T)$ yields the result.

BATTLE PLAN I – STEP 3

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- ♣ Recall that $\mathcal{R}_1 + \mathcal{R}_3 = \mathcal{R}_2 + \mathcal{R}_3 = 0$.
- ♣ Summing the equations for u_1^ε and u_3^ε and integrating in time

$$\begin{aligned} \left(u_1^\varepsilon(t, x) + u_3^\varepsilon(t, x) \right) - \operatorname{div} \left(\mathbf{D} \int_0^t (d_1 \nabla u_1^\varepsilon(s, x) + d_3 \nabla u_3^\varepsilon(s, x)) ds \right) \\ = \left(u_1^{\text{in}}(x) + u_3^{\text{in}}(x) \right) \end{aligned}$$

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- ♣ Multiply by $(d_1 u_1^\varepsilon + d_3 u_3^\varepsilon)$ and some algebra yields result.

BATTLE PLAN I – STEP 4

Proposition (Weak compactness)

The solution $u_i^\varepsilon(t, x)$ satisfies

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$$\left. \begin{array}{l} \|\nabla \sqrt{u_i^\varepsilon}\|_{L^2(\Omega_T)} \leq C \\ \|u_i^\varepsilon\|_{L^2(\Omega_T)} \leq C \end{array} \right\} \implies \|\nabla u_i^\varepsilon\|_{L^{\frac{4}{3}}(\Omega_T)} \leq C.$$

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♣ Using $\frac{3}{2}$ and 3 as Hölder conjugates, we have

$$\iint_{\Omega_T} |\nabla u_i^\varepsilon|^{\frac{4}{3}} = \iint_{\Omega_T} \frac{|\nabla u_i^\varepsilon|^{\frac{4}{3}}}{|u_i^\varepsilon|^{\frac{2}{3}}} |u_i^\varepsilon|^{\frac{2}{3}} \leq \left(\iint_{\Omega_T} \left(\frac{|\nabla u_i^\varepsilon|^{\frac{4}{3}}}{|u_i^\varepsilon|^{\frac{2}{3}}} \right)^{\frac{3}{2}} \right)^{\frac{2}{3}} \left(\iint_{\Omega_T} \left(|u_i^\varepsilon|^{\frac{2}{3}} \right)^3 \right)^{\frac{1}{3}}$$

BATTLE PLAN II – STEP 1

Proposition (Relative compactness of sums)

The families $u_1^\varepsilon + u_3^\varepsilon$ and $u_2^\varepsilon + u_3^\varepsilon$ are relatively compact in $L^{\frac{4}{3}}(\Omega_T)$.

Aubin-Lions compactness criterion

Let B_1, B_2, B_3 be Banach spaces such that $B_1 \subseteq B_2 \subseteq B_3$.

Suppose $w^\varepsilon \in L^p((0, T); B_1)$ and $\partial_t w^\varepsilon \in L^q((0, T); B_3)$ with $\frac{1}{p} + \frac{1}{q} = 1$.

Then w^ε is relatively compact in $L^p((0, T); B_2)$.

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$$\begin{aligned}
 u_1^\varepsilon + u_3^\varepsilon &\in L^{\frac{4}{3}}((0, T); W^{1, \frac{4}{3}}(\Omega)) \\
 \mathcal{R}_1 + \mathcal{R}_3 = 0 &\implies \partial_t(u_1^\varepsilon + u_3^\varepsilon) - \operatorname{div}(\mathbf{D}(d_1 \nabla u_1^\varepsilon + d_2 \nabla u_3^\varepsilon)) = 0. \\
 &\implies \partial_t(u_1^\varepsilon + u_3^\varepsilon) \in L^4((0, T); W^{-1, 4}(\Omega))
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♣ Result follows by Aubin-Lions (take $p = \frac{4}{3}$ and $q = 4$).

BATTLE PLAN II – STEP 2

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♣ Recall that for a subsequence

$$u_1^\varepsilon + u_3^\varepsilon \rightarrow S_{13} \text{ strongly in } L^{\frac{4}{3}}(\Omega_T) \text{ and a.e. in } \Omega_T$$

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♣ We can show that $u_1^\varepsilon(t, x) \rightarrow u_1^*(t, x)$ a.e. in Ω_T (**nontrivial**)

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♣ We can show that $u_1^\varepsilon(t, x) \rightarrow u_1^*(t, x)$ a.e. in Ω_T (nontrivial)

♣ Furthermore we have

$$0 \leq u_1^\varepsilon \leq u_1^\varepsilon + u_3^\varepsilon \rightarrow S_{13} \text{ strongly in } L^{\frac{4}{3}}(\Omega_T).$$

♣ Lebesgue's dominated convergence theorem then yields the result.

BATTLE PLAN II – STEP 3

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So, we should prove that $u_1^\varepsilon(t, x)$ strongly converges in $L^4(\Omega_T)$.

Proposition (Higher integrability)

The solution $u_i^\varepsilon(t, x)$ satisfies

$$\|u_i^\varepsilon\|_{L^{4+\delta}(\Omega_T)} \leq C \quad \text{for some } \delta > 0.$$

BATTLE PLAN II – STEP 3

♣ Consider the forward and backward heat equations

$$\begin{cases} \partial_t w - \Delta(\mu w) = 0 & \text{in } \Omega_T \\ w(0, x) = w^{\text{in}} & \text{in } \Omega \\ \nabla w \cdot \mathbf{n}(x) = 0 & \text{on } \partial\Omega_T \end{cases}$$

where $0 < a \leq \mu(t, x) \leq b < \infty$.

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BATTLE PLAN II – STEP 3

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$$\|w\|_{L^p(\Omega_T)} \leq C \|w^{\text{in}}\|_{L^p(\Omega)}$$

BATTLE PLAN II – STEP 3

Proposition (Higher integrability)

The solution $u_i^\varepsilon(t, x)$ satisfies

$$\|u_i^\varepsilon\|_{L^{4+\delta}(\Omega_T)} \leq C \quad \text{for some } \delta > 0.$$

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$$\partial_t (u_1^\varepsilon + u_3^\varepsilon) - d_1 \Delta u_1^\varepsilon - d_3 \Delta u_3^\varepsilon = 0$$

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- ♣ Take

$$w(t, x) := u_1^\varepsilon + u_3^\varepsilon, \quad \mu(t, x) := \frac{d_1 u_1^\varepsilon + d_3 u_3^\varepsilon}{u_1^\varepsilon + u_3^\varepsilon}$$

- ♣ Parabolic duality estimates will yield the result. 

BATTLE PLAN II – STEP 4

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Proposition (Relative compactness)

The solution families $u_i^\varepsilon(t, x)$ are relatively compact in $L^4(\Omega_T)$.

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♣ Using interpolation in L^p -spaces yields

$$\left. \begin{aligned} \lim_{\varepsilon \rightarrow 0} \|u_i^\varepsilon - u_i^*\|_{L^{\frac{4}{3}}(\Omega_T)} &= 0 \\ \|u_i^\varepsilon\|_{L^{4+\delta}(\Omega_T)} &\leq C \end{aligned} \right\} \implies \lim_{\varepsilon \rightarrow 0} \|u_i^\varepsilon - u_i^*\|_{L^4(\Omega_T)} = 0.$$

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THANK YOU